

Letters to the Editor

Indian J. Phys. **49**, 950 (1975)

The crystal structure of caesium salt of acetylene dicarboxylic acid, CsHC_4O_4 , H_2O

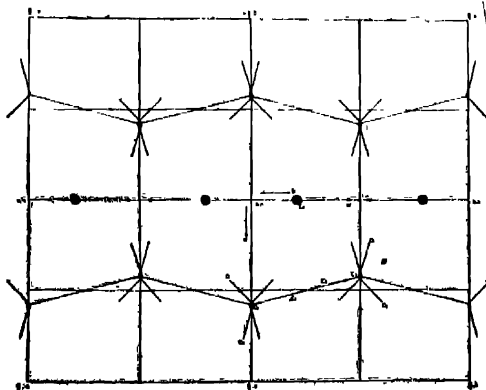
M. P. GUPTA AND A. P. MAHATA

Department of Physics, Ranchi University, Ranchi-834008.

(Received 24 March 1975).

The title compound has been investigated by us using X-ray single crystal data as part of a programme for studying hydrogen bonded solids.

The crystals are transparent, lath-like plates and are monoclinic with $a = 12.76$, $b = 7.96$, $c = 6.79 \text{ \AA}$, $\beta = 92.27^\circ$, 4 units of CsHC_4O_4 , H_2O in the unit cell. Space group is either C_2 or $C2/c$. Statistical intensity tests show hypercentric distribution in the $hk0$ data, hence $C2/c$ assumed in the present work.



The Cs and water molecule lie on special positions on the two fold axis; the organic part of the molecules occupy centres of symmetry. A view of the crystal structure down $[001]$ based on Cs phased Fourier is shown in figure 1. The structure consists of extensive chains of acetylene dicarboxylic acid residues, hydrogen bonded, parallel to the $[010]$ axis. Parallel extensive chains of molecules are cross-linked by hydrogen bonds via the water molecules.

The crystal structure is being refined to locate the hydrogen atoms which probably are so fixed as to give short symmetrical hydrogen bonds of 2.44 \AA in the structure. Atomic positions of all other atoms also are being refined and are not being reported here. The R factor at this stage of analysis is 9.4% .